



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:02 AM GMT

PDB ID : 3C8H  
Title : Crystal structure of the enterobactin esterase FES from *Shigella flexneri* in the presence of 2,3-Di-hydroxy-N-benzoyl-serine  
Authors : Kim, Y.; Maltseva, N.; Abergel, R.; Holzle, D.; Raymond, K.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2008-02-12  
Resolution : 2.48 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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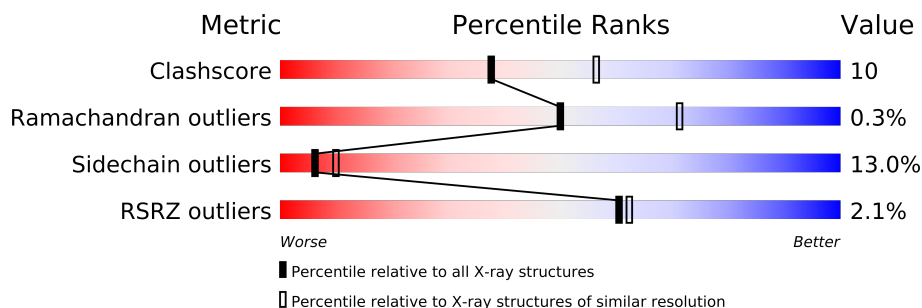
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.48 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	4136 (2.50-2.46)
Ramachandran outliers	78287	4052 (2.50-2.46)
Sidechain outliers	78261	4054 (2.50-2.46)
RSRZ outliers	66119	3279 (2.50-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	403	
1	B	403	
1	C	403	
1	D	403	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12711 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Enterochelin esterase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	Se	0	0	0
			3091	1988	543	548	5	7			
1	B	383	Total	C	N	O	S	Se	0	0	0
			3090	1987	542	549	5	7			
1	C	383	Total	C	N	O	S	Se	0	0	0
			3091	1988	543	548	5	7			
1	D	383	Total	C	N	O	S	Se	0	2	0
			3106	1996	544	554	5	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q83SB9
A	-1	ASN	-	EXPRESSION TAG	UNP Q83SB9
A	0	ALA	-	EXPRESSION TAG	UNP Q83SB9
B	-2	SER	-	EXPRESSION TAG	UNP Q83SB9
B	-1	ASN	-	EXPRESSION TAG	UNP Q83SB9
B	0	ALA	-	EXPRESSION TAG	UNP Q83SB9
C	-2	SER	-	EXPRESSION TAG	UNP Q83SB9
C	-1	ASN	-	EXPRESSION TAG	UNP Q83SB9
C	0	ALA	-	EXPRESSION TAG	UNP Q83SB9
D	-2	SER	-	EXPRESSION TAG	UNP Q83SB9
D	-1	ASN	-	EXPRESSION TAG	UNP Q83SB9
D	0	ALA	-	EXPRESSION TAG	UNP Q83SB9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	80	Total	O	0	0
			80	80		
2	B	85	Total	O	0	0
			85	85		

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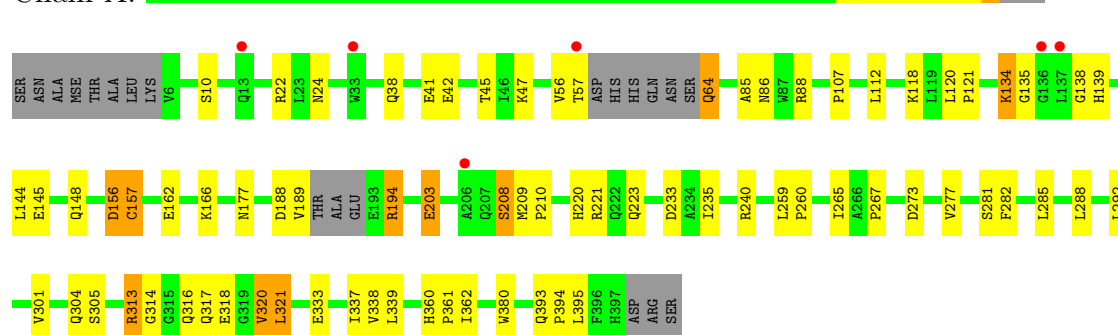
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	90	Total	O	0	0
			90	90		
2	D	78	Total	O	0	0
			78	78		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

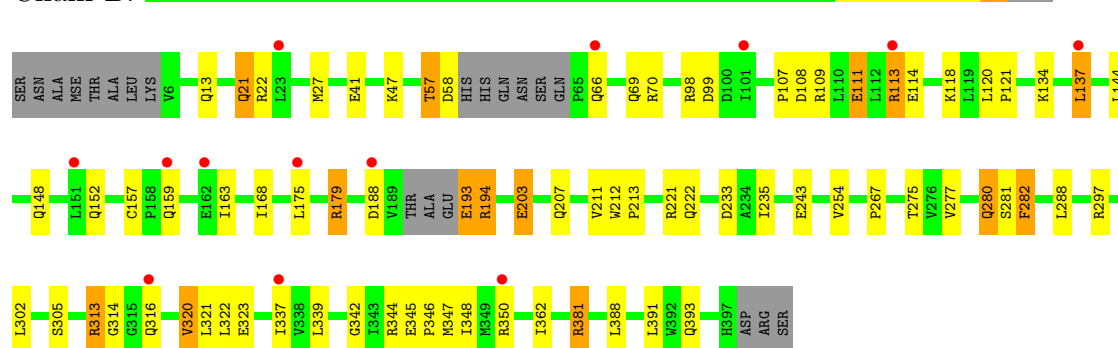
- Molecule 1: Enterochelin esterase

Chain A:



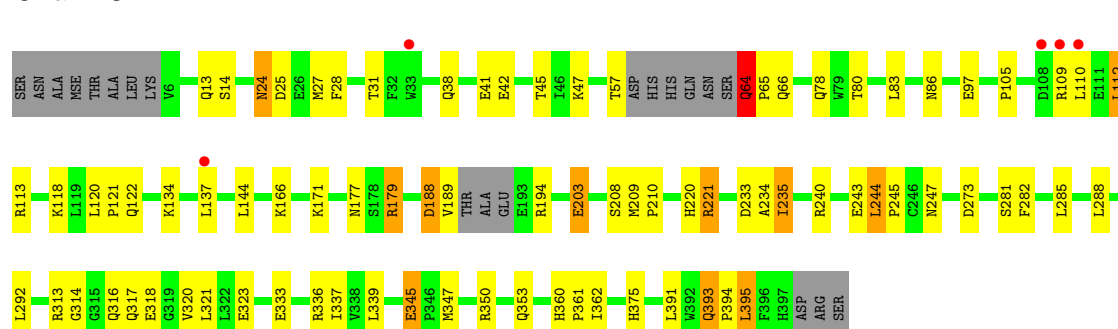
- Molecule 1: Enterochelin esterase

Chain B:



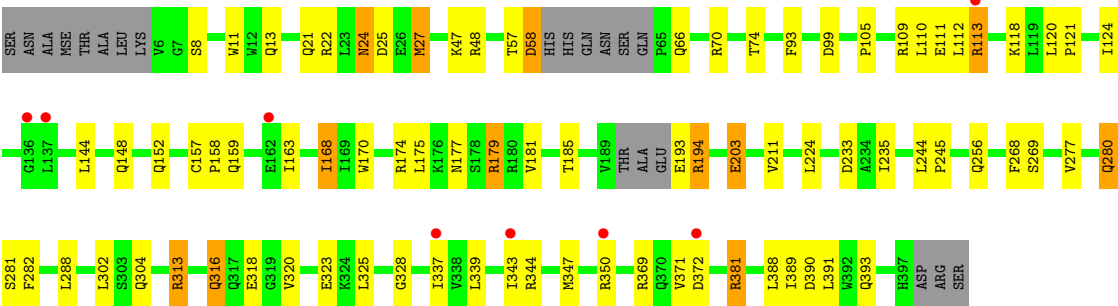
- Molecule 1: Enterochelin esterase

Chain C:



● Molecule 1: Enterochelin esterase

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.51Å 48.78Å 156.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.23 – 2.48 47.23 – 2.48	Depositor EDS
% Data completeness (in resolution range)	94.2 (47.23-2.48) 94.2 (47.23-2.48)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.183 , 0.225 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	40.5	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.7	EDS
Estimated twinning fraction	0.429 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 57022 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12711	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.37 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.7823e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.49	1/3184 (0.0%)	0.57	1/4334 (0.0%)
1	B	0.46	0/3183	0.56	0/4332
1	C	0.48	0/3184	0.59	2/4334 (0.0%)
1	D	0.50	0/3198	0.59	0/4351
All	All	0.48	1/12749 (0.0%)	0.58	3/17351 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	THR	C-O	7.07	1.36	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	GLN	N-CA-C	-5.89	95.10	111.00
1	C	64	GLN	N-CA-C	-5.36	96.53	111.00
1	C	112	LEU	CA-CB-CG	-5.16	103.42	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	B	314	GLY	Peptide
1	C	345	GLU	Peptide

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3091	0	0	34	0
1	B	3090	0	0	33	0
1	C	3091	0	0	30	0
1	D	3106	0	0	33	0
2	A	80	0	0	5	0
2	B	85	0	0	6	0
2	C	90	0	0	2	0
2	D	78	0	0	3	0
All	All	12711	0	0	124	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (124) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:152:GLN:OE1	1:B:381:ARG:CD	2.22	0.88
1:B:179:ARG:NH2	1:B:243:GLU:OE1	2.18	0.77
1:A:22:ARG:CG	1:A:24:ASN:O	2.36	0.74
1:C:347:MSE:SE	1:D:313:ARG:NH1	2.73	0.71
1:B:221:ARG:O	1:B:222:GLN:CG	2.39	0.70
1:C:360:HIS:N	1:C:361:PRO:CD	2.55	0.69
1:C:57:THR:O	1:C:57:THR:CG2	2.40	0.69
1:B:22:ARG:NH1	1:B:148:GLN:NE2	2.42	0.67
1:D:22:ARG:NH1	1:D:148:GLN:NE2	2.42	0.67
1:D:369:ARG:NH2	1:D:390:ASP:OD1	2.29	0.66
1:D:304:GLN:NE2	2:D:410:HOH:O	2.28	0.66
1:A:317:GLN:NE2	1:B:137:LEU:CG	2.59	0.66
1:B:57:THR:O	1:B:58:ASP:C	2.33	0.65
1:C:41:GLU:N	1:C:41:GLU:OE1	2.29	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:360:HIS:N	1:A:361:PRO:CD	2.60	0.65
1:A:138:GLY:N	2:A:479:HOH:O	2.28	0.65
1:B:281:SER:OG	1:B:282:PHE:N	2.30	0.65
1:A:139:HIS:CE1	2:A:419:HOH:O	2.51	0.64
1:A:316:GLN:NE2	2:A:427:HOH:O	2.32	0.61
1:B:22:ARG:NH2	1:B:148:GLN:NE2	2.49	0.61
1:C:24:ASN:OD1	1:C:27:MSE:CB	2.51	0.59
1:C:244:LEU:N	1:C:245:PRO:CD	2.67	0.58
1:A:188:ASP:O	1:A:189:VAL:CB	2.52	0.57
1:D:109:ARG:NH2	2:D:444:HOH:O	2.36	0.57
1:D:57:THR:O	1:D:58:ASP:C	2.43	0.56
1:C:233:ASP:OD2	1:C:235:ILE:N	2.38	0.56
1:C:233:ASP:OD2	1:C:234:ALA:N	2.38	0.56
1:C:336:ARG:NH2	1:C:391:LEU:O	2.38	0.56
1:C:393:GLN:N	1:C:394:PRO:CD	2.69	0.56
1:A:203:GLU:CG	1:A:233:ASP:OD2	2.52	0.56
1:C:38:GLN:NE2	1:C:45:THR:N	2.53	0.55
1:C:179:ARG:NH2	1:C:243:GLU:OE1	2.39	0.55
1:D:316:GLN:CA	1:D:316:GLN:NE2	2.69	0.55
1:B:21:GLN:NE2	2:B:455:HOH:O	2.40	0.55
1:D:48:ARG:NH2	2:D:417:HOH:O	2.39	0.54
1:D:371:VAL:CG1	1:D:372:ASP:N	2.70	0.54
1:C:188:ASP:O	1:C:189:VAL:CB	2.55	0.54
1:A:320:VAL:CG1	1:A:321:LEU:N	2.71	0.54
1:D:203:GLU:CG	1:D:233:ASP:OD2	2.55	0.53
1:B:69:GLN:NE2	2:B:482:HOH:O	2.41	0.53
1:A:120:LEU:N	1:A:121:PRO:CD	2.71	0.53
1:A:317:GLN:NE2	1:B:137:LEU:CD2	2.72	0.53
1:C:221:ARG:NH2	2:C:417:HOH:O	2.42	0.52
1:C:350:ARG:NH1	1:C:353:GLN:NE2	2.58	0.52
1:C:203:GLU:CG	1:C:233:ASP:OD2	2.58	0.52
1:B:70:ARG:NH2	2:B:462:HOH:O	2.44	0.51
1:C:31:THR:OG1	1:C:80:THR:OG1	2.28	0.51
1:A:38:GLN:NE2	1:A:45:THR:N	2.59	0.51
1:D:24:ASN:ND2	1:D:27:MSE:N	2.59	0.50
1:D:185[A]:THR:CG2	1:D:194:ARG:NH2	2.74	0.50
1:B:98:ARG:NH2	2:B:413:HOH:O	2.43	0.50
1:C:345:GLU:OE2	1:C:375:HIS:ND1	2.44	0.50
1:B:280:GLN:O	1:B:281:SER:OG	2.30	0.50
1:B:203:GLU:CG	1:B:233:ASP:OD2	2.60	0.49
1:A:41:GLU:OE1	1:A:41:GLU:N	2.46	0.49
1:D:120:LEU:N	1:D:121:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:259:LEU:N	1:A:260:PRO:CD	2.75	0.49
1:D:281:SER:OG	1:D:282:PHE:N	2.46	0.49
1:B:120:LEU:N	1:B:121:PRO:CD	2.77	0.47
1:A:313:ARG:CG	1:B:313:ARG:CB	2.92	0.47
1:A:305:SER:OG	1:A:380:TRP:NE1	2.47	0.47
1:D:152:GLN:OE1	1:D:381:ARG:CD	2.63	0.47
1:B:99:ASP:C	1:B:99:ASP:OD2	2.52	0.47
1:C:97:GLU:OE1	1:C:122:GLN:NE2	2.47	0.47
1:A:85:ALA:O	1:A:148:GLN:N	2.48	0.47
1:B:346:PRO:CD	2:B:421:HOH:O	2.63	0.47
1:B:41:GLU:OE1	1:B:41:GLU:N	2.47	0.47
1:B:342:GLY:N	1:B:345:GLU:OE1	2.48	0.47
1:C:247:ASN:C	1:C:247:ASN:OD1	2.53	0.47
1:C:314:GLY:O	1:D:113:ARG:CG	2.63	0.47
1:D:157:CYS:N	1:D:158:PRO:CD	2.77	0.46
1:A:86:ASN:OD1	1:A:86:ASN:C	2.54	0.46
1:C:120:LEU:N	1:C:121:PRO:CD	2.78	0.46
1:C:395:LEU:CD2	1:C:395:LEU:N	2.78	0.46
1:A:313:ARG:NH2	1:A:313:ARG:CB	2.79	0.46
1:C:171:LYS:N	2:C:423:HOH:O	2.47	0.46
1:C:64:GLN:NE2	1:C:105:PRO:O	2.49	0.46
1:A:304:GLN:NE2	2:A:446:HOH:O	2.49	0.46
1:A:316:GLN:CG	1:A:317:GLN:N	2.79	0.45
1:D:280:GLN:O	1:D:281:SER:OG	2.35	0.45
1:A:301:VAL:O	1:A:338:VAL:N	2.49	0.45
1:D:112:LEU:O	1:D:113:ARG:C	2.55	0.45
1:D:170:TRP:CE3	1:D:179:ARG:CD	3.00	0.45
1:D:268:PHE:N	1:D:268:PHE:CD1	2.84	0.45
1:B:194:ARG:NH1	1:B:267:PRO:O	2.50	0.44
1:A:393:GLN:N	1:A:394:PRO:CD	2.80	0.44
1:B:107:PRO:CB	1:B:111:GLU:CD	2.85	0.44
1:C:244:LEU:CB	1:C:245:PRO:CD	2.96	0.44
1:C:86:ASN:OD1	1:C:86:ASN:C	2.57	0.44
1:A:135:GLY:O	2:A:479:HOH:O	2.20	0.43
1:D:99:ASP:OD2	1:D:99:ASP:C	2.55	0.43
1:B:109:ARG:NH1	1:B:113:ARG:CZ	2.81	0.43
1:A:157:CYS:SG	1:A:221:ARG:NH2	2.92	0.43
1:A:156:ASP:OD1	1:A:157:CYS:SG	2.77	0.42
1:A:209:MSE:O	1:A:210:PRO:C	2.57	0.42
1:D:177:ASN:OD1	1:D:179:ARG:NH1	2.52	0.42
1:A:240:ARG:NH1	1:A:282:PHE:CD2	2.87	0.42
1:B:157:CYS:SG	1:B:221:ARG:NH2	2.93	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:168:ILE:O	1:D:181:VAL:N	2.52	0.42
1:B:320:VAL:CG1	1:B:321:LEU:N	2.81	0.42
1:C:203:GLU:OE2	1:C:234:ALA:N	2.52	0.42
1:C:209:MSE:O	1:C:210:PRO:C	2.58	0.42
1:D:70:ARG:NH1	1:D:74:THR:O	2.53	0.41
1:B:22:ARG:CZ	1:B:148:GLN:NE2	2.83	0.41
1:B:193:GLU:N	2:B:430:HOH:O	2.53	0.41
1:A:56:VAL:CG1	1:A:56:VAL:O	2.68	0.41
1:A:88:ARG:NE	1:A:145:GLU:OE1	2.53	0.41
1:B:212:TRP:CB	1:B:213:PRO:CD	2.97	0.41
1:D:325:LEU:O	1:D:328:GLY:N	2.53	0.41
1:D:244:LEU:N	1:D:245:PRO:CD	2.84	0.41
1:C:240:ARG:NH1	1:C:282:PHE:CD2	2.88	0.41
1:A:107:PRO:CB	1:A:112:LEU:CD1	2.99	0.41
1:D:343:ILE:CG1	1:D:372:ASP:O	2.68	0.41
1:B:222:GLN:O	1:B:222:GLN:CG	2.66	0.41
1:A:314:GLY:O	1:B:113:ARG:CG	2.67	0.41
1:B:362:ILE:CG2	1:B:362:ILE:O	2.69	0.41
1:D:194:ARG:O	1:D:269:SER:N	2.54	0.41
1:D:8:SER:O	1:D:11:TRP:N	2.54	0.41
1:D:224:LEU:CD2	1:D:389:ILE:CG1	2.99	0.41
1:A:194:ARG:NH1	1:A:267:PRO:O	2.53	0.41
1:D:174:ARG:NH2	1:D:256:GLN:NE2	2.68	0.40
1:D:93:PHE:O	1:D:124:ILE:N	2.54	0.40
1:A:134:LYS:O	1:A:208:SER:OG	2.39	0.40
1:B:275:THR:OG1	1:B:297:ARG:NH2	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	377/403 (94%)	358 (95%)	18 (5%)	1 (0%)	50 71
1	B	377/403 (94%)	361 (96%)	15 (4%)	1 (0%)	50 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	377/403 (94%)	358 (95%)	18 (5%)	1 (0%)	50 71
1	D	379/403 (94%)	355 (94%)	22 (6%)	2 (0%)	38 59
All	All	1510/1612 (94%)	1432 (95%)	73 (5%)	5 (0%)	50 71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	235	ILE
1	A	235	ILE
1	D	235	ILE
1	B	235	ILE
1	D	105	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	324/333 (97%)	291 (90%)	33 (10%)	11 18
1	B	324/333 (97%)	277 (86%)	47 (14%)	5 7
1	C	324/333 (97%)	276 (85%)	48 (15%)	4 7
1	D	326/333 (98%)	286 (88%)	40 (12%)	7 11
All	All	1298/1332 (97%)	1130 (87%)	168 (13%)	6 10

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	42	GLU
1	A	47	LYS
1	A	64	GLN
1	A	118	LYS
1	A	134	LYS
1	A	144	LEU
1	A	156	ASP
1	A	157	CYS

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Mol	Chain	Res	Type
1	A	162	GLU
1	A	166	LYS
1	A	177	ASN
1	A	194	ARG
1	A	203	GLU
1	A	208	SER
1	A	220	HIS
1	A	223	GLN
1	A	265	ILE
1	A	273	ASP
1	A	277	VAL
1	A	281	SER
1	A	285	LEU
1	A	288	LEU
1	A	292	LEU
1	A	313	ARG
1	A	318	GLU
1	A	320	VAL
1	A	321	LEU
1	A	333	GLU
1	A	337	ILE
1	A	339	LEU
1	A	362	ILE
1	A	395	LEU
1	B	13	GLN
1	B	21	GLN
1	B	27	MSE
1	B	47	LYS
1	B	57	THR
1	B	66	GLN
1	B	108	ASP
1	B	111	GLU
1	B	113	ARG
1	B	114	GLU
1	B	118	LYS
1	B	134	LYS
1	B	137	LEU
1	B	144	LEU
1	B	159	GLN
1	B	163	ILE
1	B	168	ILE
1	B	175	LEU

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Mol	Chain	Res	Type
1	B	179	ARG
1	B	188	ASP
1	B	193	GLU
1	B	194	ARG
1	B	203	GLU
1	B	207	GLN
1	B	211	VAL
1	B	254	VAL
1	B	277	VAL
1	B	280	GLN
1	B	282	PHE
1	B	288	LEU
1	B	302	LEU
1	B	305	SER
1	B	313	ARG
1	B	316	GLN
1	B	320	VAL
1	B	322	LEU
1	B	323	GLU
1	B	337	ILE
1	B	339	LEU
1	B	344	ARG
1	B	347	MSE
1	B	348	ILE
1	B	350	ARG
1	B	381	ARG
1	B	388	LEU
1	B	391	LEU
1	B	393	GLN
1	C	13	GLN
1	C	14	SER
1	C	24	ASN
1	C	25	ASP
1	C	28	PHE
1	C	42	GLU
1	C	47	LYS
1	C	64	GLN
1	C	65	PRO
1	C	66	GLN
1	C	78	GLN
1	C	83	LEU
1	C	109	ARG

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Mol	Chain	Res	Type
1	C	110	LEU
1	C	112	LEU
1	C	113	ARG
1	C	118	LYS
1	C	134	LYS
1	C	137	LEU
1	C	144	LEU
1	C	166	LYS
1	C	177	ASN
1	C	179	ARG
1	C	188	ASP
1	C	194	ARG
1	C	203	GLU
1	C	208	SER
1	C	220	HIS
1	C	221	ARG
1	C	244	LEU
1	C	273	ASP
1	C	281	SER
1	C	285	LEU
1	C	288	LEU
1	C	292	LEU
1	C	313	ARG
1	C	316	GLN
1	C	317	GLN
1	C	318	GLU
1	C	320	VAL
1	C	321	LEU
1	C	323	GLU
1	C	333	GLU
1	C	337	ILE
1	C	339	LEU
1	C	362	ILE
1	C	393	GLN
1	C	395	LEU
1	D	13	GLN
1	D	21	GLN
1	D	24	ASN
1	D	25	ASP
1	D	27	MSE
1	D	47	LYS
1	D	58	ASP

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Mol	Chain	Res	Type
1	D	66	GLN
1	D	110	LEU
1	D	111	GLU
1	D	113	ARG
1	D	118	LYS
1	D	144	LEU
1	D	159	GLN
1	D	163	ILE
1	D	168	ILE
1	D	175	LEU
1	D	179	ARG
1	D	193	GLU
1	D	194	ARG
1	D	203	GLU
1	D	211	VAL
1	D	277	VAL
1	D	280	GLN
1	D	288	LEU
1	D	302	LEU
1	D	313	ARG
1	D	316	GLN
1	D	318	GLU
1	D	320	VAL
1	D	323	GLU
1	D	337	ILE
1	D	339	LEU
1	D	344	ARG
1	D	347	MSE
1	D	350	ARG
1	D	381	ARG
1	D	388	LEU
1	D	391	LEU
1	D	393	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	383/403 (95%)	0.03	6 (1%) 68 70	23, 58, 98, 118	5 (1%)
1	B	383/403 (95%)	0.06	13 (3%) 43 44	27, 56, 93, 120	11 (2%)
1	C	383/403 (95%)	-0.16	5 (1%) 74 75	24, 49, 85, 119	5 (1%)
1	D	383/403 (95%)	-0.12	8 (2%) 60 62	17, 49, 92, 114	11 (2%)
All	All	1532/1612 (95%)	-0.05	32 (2%) 60 62	17, 53, 95, 120	32 (2%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	ILE	6.5
1	B	101	ILE	5.6
1	B	162	GLU	4.7
1	D	136	GLY	4.5
1	D	113	ARG	4.2
1	C	109	ARG	4.0
1	C	110	LEU	3.7
1	B	350	ARG	3.6
1	D	137	LEU	3.5
1	B	66	GLN	3.5
1	B	113	ARG	3.2
1	B	151	LEU	3.2
1	B	137	LEU	3.1
1	D	372	ASP	3.0
1	C	137	LEU	3.0
1	B	23	LEU	2.8
1	B	159	GLN	2.8
1	D	343	ILE	2.8
1	A	137	LEU	2.7
1	B	188	ASP	2.7
1	D	337	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	206	ALA	2.4
1	C	108	ASP	2.4
1	A	33	TRP	2.3
1	D	162	GLU	2.2
1	C	33	TRP	2.1
1	B	175	LEU	2.1
1	B	316	GLN	2.1
1	A	136	GLY	2.1
1	D	350	ARG	2.0
1	A	13	GLN	2.0
1	A	57	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.